10/070643

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L7 4 SEA SSS FUL L6

to overcome 09/10/1999

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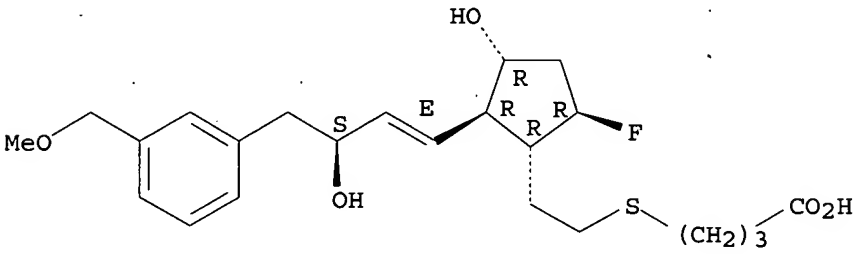
L7 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2003 ACS on STN
RN 256382-26-0 REGISTRY
CN Butanoic acid, 4-[[2-[(1R,2R,3R,5R)-5-fluoro-3-hydroxy-2-[(1E,3S)-3-hydroxy-4-[3-(methoxymethyl)phenyl]-1-butenyl]cyclopentyl]ethyl]thio]-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H33 F O5 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.

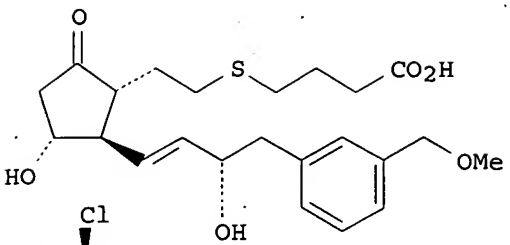


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1947 TO DATE)
3 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1

AN 137:109132 CA
TI Design and synthesis of a selective EP4-receptor agonist. Part 3: 16-phenyl-5-thiaPGE1 and 9-.beta.-halo derivatives with improved stability
AU Maruyama, Toru; Asada, Masaki; Shiraishi, Tai; Yoshida, Hideyuki; Maruyama, Takayuki; Ohuchida, Shuichi; Nakai, Hisao; Kondo, Kigen; Toda, Masaaki
CS Minase Research Institute, Ono Pharmaceutical Co., Ltd., Shimamoto, Mishima, Osaka, 618-8585, Japan
SO Bioorganic & Medicinal Chemistry (2002), 10(6), 1743-1759
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
GI



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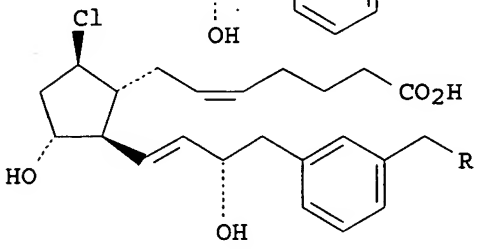


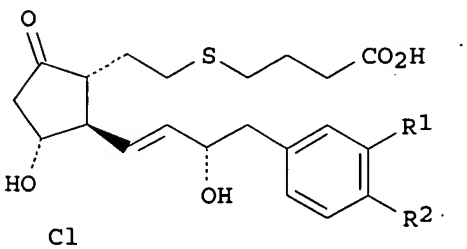
II

AB To identify a new selective EP4-agonist with improved chem. stability, further chem. modification of those reported previously was continued. We focused our attention on chem. modification of the .alpha. chain of 3,7-dithiaPGE1 and selected 5-thiaPGE1 as a new chem. lead. Introduction of an optimized .omega. chain to the 5-thiaPG skeleton afforded m-methoxymethyl deriv. I, which showed the most potent EP4-receptor agonist activity and good subtype-selectivity both in vitro and in vivo. 9.beta.-HaloPGF derivs. were also synthesized and biol. evaluated in an attempt to block self-degrdn. of the .beta.-hydroxyketone moiety. Among these series, II (R1 = OMe, OEt) showed potent agonist activity and good subtype-selectivity. Structure-activity relationships (SARs) are also discussed.

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 135:327477 CA
TI Design and synthesis of a highly selective EP4-receptor agonist. Part 2. 5-Thia and 9.beta.-halo-PG derivatives with improved stability
AU Maruyama, T.; Asada, M.; Shiraishi, T.; Sakata, K.; Seki, A.; Yoshida, H.; Shinagawa, Y.; Maruyama, T.; Ohuchida, S.; Nakai, H.; Kondo, K.; Toda, M.
CS Minase Research Institute, Ono Pharmaceutical Co., Ltd., Shimamoto, Mishima, Osaka, 618-8585, Japan
SO Bioorganic & Medicinal Chemistry Letters (2001), 11(15), 2033-2035
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
GI



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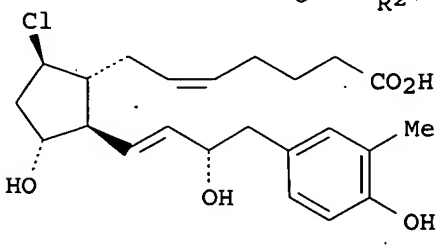

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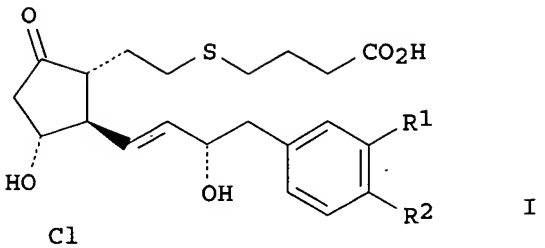

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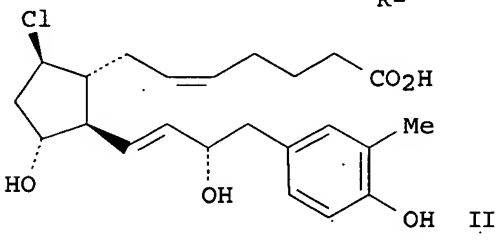

II

AB EP prostanoid receptor binding structure-activity relationships of 5-thia- and 9.beta.-halo-prostaglandins were evaluated. 5-Thia-PGE1 I (R1 = CH2OMe, R2 = H; R1 = Me, R2 = Y) and 9.beta.-chloro-PGF2 II were shown to be EP4-receptor selective agonists.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 3

AN 132:122442 CA

TI Preparation of 5-thia-.omega.-substituted phenyl-prostaglandin derivatives with binding affinity to prostaglandin E2 (PEG2) receptors

IN Maruyama, Toru; Ohuchida, Shuichi

PA Ono Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 84 pp.
CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000003980	A1	20000127	WO 1999-JP3798	19990714
	W: AU, BR, CA, CN, HU, JP, KR, MX, NO, NZ, RU, TR, US, ZA				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2336952	AA	20000127	CA 1999-2336952	19990714
	AU 9946518	A1	20000207	AU 1999-46518	19990714
	JP 2001089444	A2	20010403	JP 2000-104840	19990714
	BR 9912813	A	20010502	BR 1999-12813	19990714
	EP 1097922	A1	20010509	EP 1999-929831	19990714
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 3174563	B2	20010611	JP 1989-5600	19990714
	NZ 509293	A	20030530	NZ 1999-509293	19990714
	US 6462081	B1	20021008	US 2000-720675	20001229
	NO 2001000213	A	20010315	NO 2001-213	20010112
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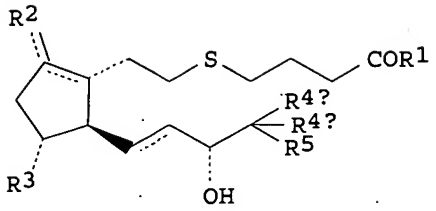

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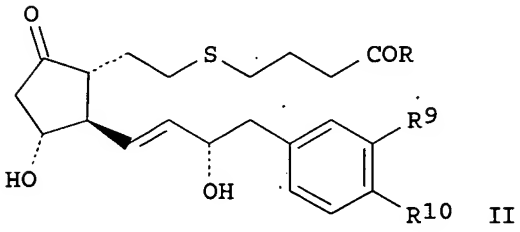


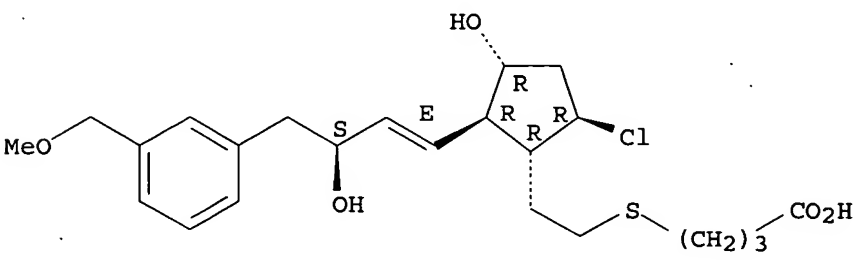
II

AB 5-Thia-.omega.-substituted phenyl-prostaglandin E derivs. represented by general formula (I; R1 = HO, C1-6 alkoxy, NR6R7; R6, R7 = H, C1-4 alkyl; R2 = oxo, halo, O2CR8; R8 = C1-4 alkyl, Ph, phenyl-C1-4 alkyl; R3 = H, HO; R4a, R4b = H,C1-4 alkyl; R5 = substituted Ph; the solid line accompanied by dotted line represents a single or double bond, provided that when R2 = O2CR8, the 8-9 position possesses a double bonds.) are prepd. Because of being capable of bonding strongly to PEG2 receptors (in particular, the subtype EP4), the compds. represented by general formula I are expected as useful in preventing and/or treating immunol. diseases, asthma, bone dysplasia, nerve cell death, lung injury, hepatopathy, acute hepatitis, nephritis, renal insufficiency, hypertension, myocardial ischemia, systemic inflammatory syndrome, ambustion pain, sepsis, hemophagous syndrome, macrophage activation syndrome, Still disease, Kawasaki disease, burn, systemic granulomatosis, ulcerative colitis, Crohn's disease, hypercytokinemia at dialysis, multiple organ failure, shock, etc. Moreover, PEG2 receptors participate in sleep disorders and platelet aggregation and, therefore, these compds. are expected as useful in preventing/treating these diseases. The title compd. (II; R = OH, R9 = Me, R10 = OH) exhibited affinity to mouse EP4, EP1, and EP3.alpha. receptors with Ki of 0.0024, >10, and 2.9, resp., in CHO cells expressing these prostanoid receptor subtypes. A tablet and vial formulation contg. II (R = OMe, R9 = CH2OMe, R10 = H) were described.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2003 ACS on STN
RN 256382-25-9 REGISTRY
CN Butanoic acid, 4-[[2-[(1R,2R,3R,5R)-5-chloro-3-hydroxy-2-[(1E,3S)-3-hydroxy-4-[3-(methoxymethyl)phenyl]-1-butenyl]cyclopentyl]ethyl]thio]-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H33 Cl O5 S
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1

AN 132:122442 CA
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IN Maruyama, Toru; Ohuchida, Shuichi
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000003980	A1	20000127	WO 1999-JP3798	19990714
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RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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NZ 509293	A	20030530	NZ 1999-509293	19990714
US 6462081	B1	20021008	US 2000-720675	20001229
NO 2001000213	A	20010315	NO 2001-213	20010112
PRAI JP 1998-200752	19980715			
JP 2000-560089	19990714			
WO 1999-JP3798	19990714			

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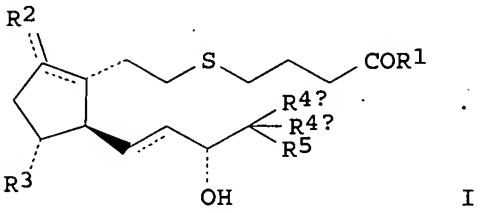

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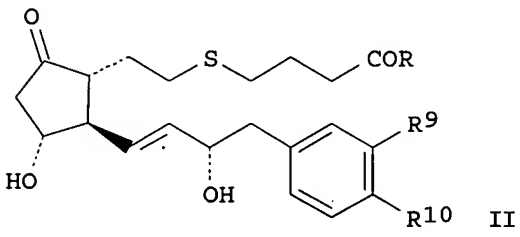

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RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
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L7 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2003 ACS on STN
RN 256382-22-6 REGISTRY
CN Butanoic acid, 4-[[2-[(1R,2R,3R,5R)-5-fluoro-3-hydroxy-2-[(1E,3S)-3-hydroxy-4-[3-(methoxymethyl)phenyl]-1-butenyl]cyclopentyl]ethyl]thio]-, methyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H35 F O5 S
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LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

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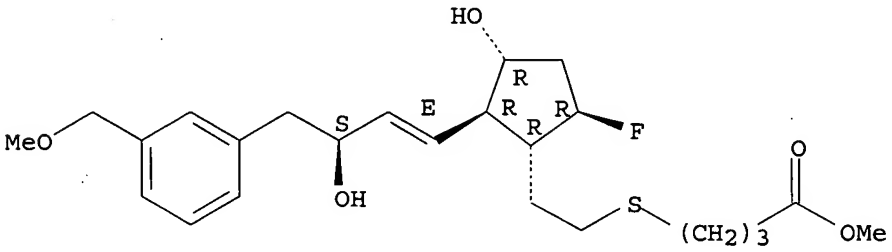
Double bond geometry as shown.



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CS Minase Research Institute, Ono Pharmaceutical Co., Ltd., Shimamoto, Mishima, Osaka, 618-8585, Japan
SO Bioorganic & Medicinal Chemistry (2002), 10(6), 1743-1759
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
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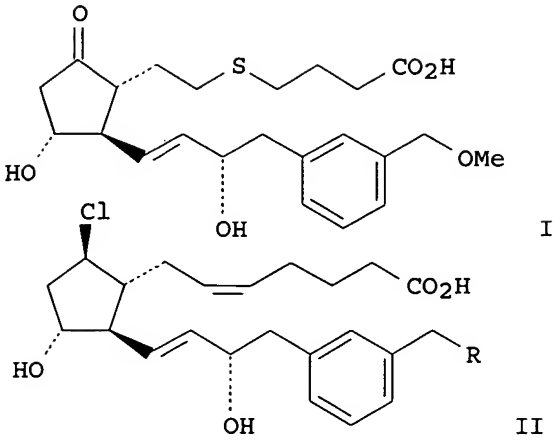

I

II

AB To identify a new selective EP4-agonist with improved chem. stability, further chem. modification of those reported previously was continued. We focused our attention on chem. modification of the .alpha. chain of 3,7-dithiaPGE1 and selected 5-thiaPGE1 as a new chem. lead. Introduction of an optimized .omega. chain to the 5-thiaPG skeleton afforded m-methoxymethyl deriv. I, which showed the most potent EP4-receptor agonist activity and good subtype-selectivity both in vitro and in vivo. 9.beta.-HaloPGF derivs. were also synthesized and biol. evaluated in an attempt to block self-degrdn. of the .beta.-hydroxyketone moiety. Among these series, II (R1 = OMe, OEt) showed potent agonist activity and good subtype-selectivity. Structure-activity relationships (SARs) are also discussed.

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REFERENCE 2

AN 132:122442 CA
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IN Maruyama, Toru; Ohuchida, Shuichi
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000003980	A1	20000127	WO 1999-JP3798	19990714
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	AU 9946518	A1	20000207	AU 1999-46518	19990714
	JP 2001089444	A2	20010403	JP 2000-104840	19990714
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	EP 1097922	A1	20010509	EP 1999-929831	19990714
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	NZ 509293	A	20030530	NZ 1999-509293	19990714
	US 6462081	B1	20021008	US 2000-720675	20001229
	NO 2001000213	A	20010315	NO 2001-213	20010112
PRAI	JP 1998-200752	19980715			
	JP 2000-560089	19990714			
	WO 1999-JP3798	19990714			

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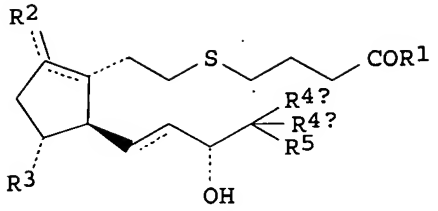

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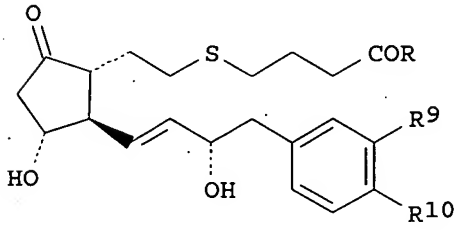

II

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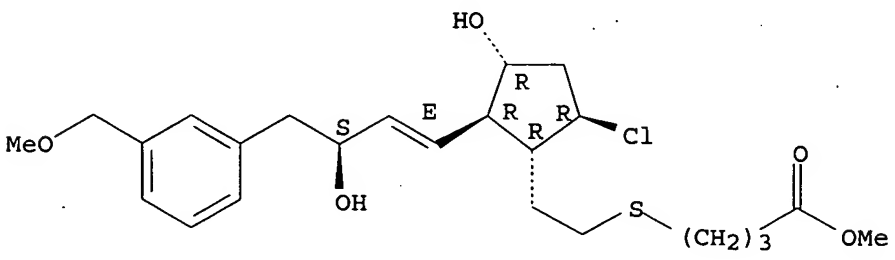
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2003 ACS on STN
RN 256382-21-5 REGISTRY
CN Butanoic acid, 4-[[2-[(1R,2R,3R,5R)-5-chloro-3-hydroxy-2-[(1E,3S)-3-hydroxy-4-[3-(methoxymethyl)phenyl]-1-butenyl]cyclopentyl]ethyl]thio]-, methyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H35 Cl O5 S
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

REFERENCE 1

AN 132:122442 CA
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IN Maruyama, Toru; Ohuchida, Shuichi
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000003980	A1	20000127	WO 1999-JP3798	19990714
	W: AU, BR, CA, CN, HU, JP, KR, MX, NO, NZ, RU, TR, US, ZA				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2336952	AA	20000127	CA 1999-2336952	19990714
	AU 9946518	A1	20000207	AU 1999-46518	19990714
	JP 2001089444	A2	20010403	JP 2000-104840	19990714
	BR 9912813	A	20010502	BR 1999-12813	19990714
	EP 1097922	A1	20010509	EP 1999-929831	19990714
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	US 6462081	B1	20021008	US 2000-720675	20001229
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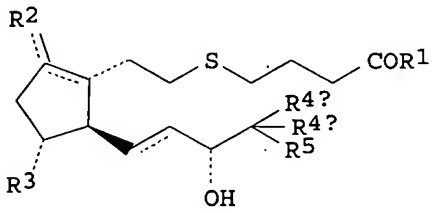

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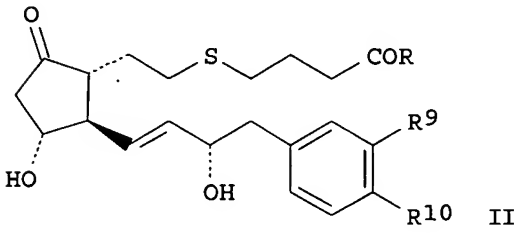

II

AB 5-Thia-.omega.-substituted phenyl-prostaglandin E derivs. represented by general formula (I; R1 = HO, C1-6 alkoxy, NR6R7; R6, R7 = H, C1-4 alkyl; R2 = oxo, halo, O2CR8; R8 = C1-4 alkyl, Ph, phenyl-C1-4 alkyl; R3 = H, HO; R4a, R4b = H,C1-4 alkyl; R5 = substituted Ph; the solid line accompanied by dotted line represents a single or double bond, provided that when R2 = O2CR8, the 8-9 position possesses a double bonds.) are prepd. Because of being capable of bonding strongly to PEG2 receptors (in particular, the subtype EP4), the compds. represented by general formula I are expected as useful in preventing and/or treating immunol. diseases, asthma, bone dysplasia, nerve cell death, lung injury, hepatopathy, acute hepatitis,

nephritis, renal insufficiency, hypertension, myocardial ischemia, systemic inflammatory syndrome, ambustion pain, sepsis, hemophagous syndrome, macrophage activation syndrome, Still disease, Kawasaki disease, burn, systemic granulomatosis, ulcerative colitis, Crohn's disease, hypercytokinemia at dialysis, multiple organ failure, shock, etc. Moreover, PEG2 receptors participate in sleep disorders and platelet aggregation and, therefore, these compds. are expected as useful in preventing/treating these diseases. The title compd. (II; R = OH, R9 = Me, R10 = OH) exhibited affinity to mouse EP4, EP1, and EP3.alpha. receptors with Ki of 0.0024, >10, and 2.9, resp., in CHO cells expressing these prostanoid receptor subtypes. A tablet and vial formulation contg. II (R = OMe, R9 = CH2OMe, R10 = H) were described.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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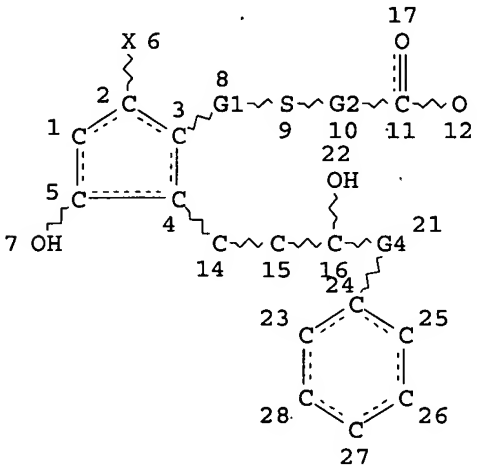

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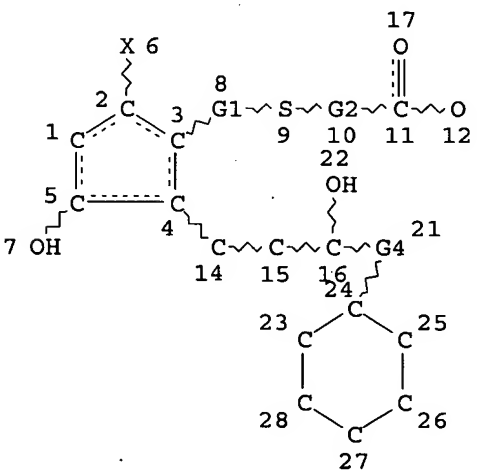

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FULL SCREEN SEARCH COMPLETED - . 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L8

=>

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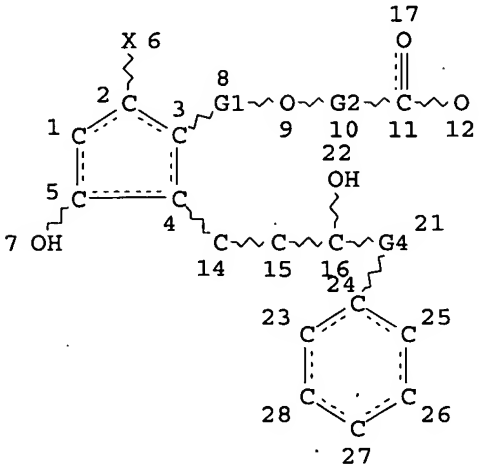


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L13            0 SEA SSS FUL L12

=>
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